Changes to BatPaC for Version 3.0

Introduction

The BatPaC model Version 1.0 and a descriptive manual that provided instructions for its use was first distributed in November 2011. That version of BatPaC was updated to Version 2.0 and the Manual (ANL-12/55) was revised and they were distributed in December 2012. Several minor revisions followed with brief description of the changes.

This new version of BatPaC provides several improvements, and the Manual is being revised and will be distributed early in 2016. The major changes and additions to BatPaC are briefly described below in discussions of the BatPaC worksheets.

Chem Worksheet

The positive electrode material NMC441 has been replaced by NMC622, which is the more commonly cited, and a mixed electrode material NMC/x%LMO, with any desired value of x, has been added.

Other additions are (1) sustained power parameters, (2) ASI values for 30-sec burst power, and (3) lithium content parameters for the electrodes and electrolyte.

The specific capacities of the electrodes and the thicknesses of the current collector foils and the separator have been changed in response to recent reported improvements.

The cost of some of the positive active materials has been updated by modeling of a co-precipitation based production process for NMC and NCA materials. The cost of the raw materials, sulfates of nickel, manganese, and cobalt were estimated based on the metal commodity prices, e.g., the cost of a mole of nickel sulfate = cost of a g-atom of nickel, etc. For a base case set of input parameters and assumptions, the cost of all raw materials represented ~50% of the cost of the final NMC333 product. The new estimates are:
NMC333 : $20/kg (previously $31)
$Ni_{0.8}Co_{0.15}Al_{0.05}$: $24/kg (previously $33)

The cost of the graphite (negative active material) has been changed to $15/kg (previously $19/kg).

The power factor for the active materials has been lowered from 0.95 to 0.90, which results in a greater reduction in the unit cost of these materials with increasing scale of production.

Battery Design

The color scheme has been changed for denoting default input values that may be changed and for battery design inputs that the user is required to make.

The default value of the cell thickness for EV batteries has been increased from 12 mm to 20mm. For all vehicle types, the model automatically adjusts slightly the cell thickness to provide whole numbers of bicell layers, rather than allowing partial layers as in BatPaC 2.0.

The calculation of the electrode coating thickness has been revised to include limits on thickness imposed by sustained discharges, which sometimes results in thinner than calculated from the area needed to provide the designated power. The resulting thickness may be further reduced by the user, for instance to improve battery efficiency and cold-weather performance or to increase the maximum rate of charging.

The overall improvement in the estimated maximum thickness of the electrode coating, often results in thinner coatings than those calculated by BatPaC 2.0 and rarely reaches 100 microns. As a result, the previous arbitrary limit on coating thickness of 100 microns has been eliminated.

The new version adds a calculation of the lithium requirement per battery pack to assist in studies of long-term lithium requirements for the electric-drive vehicle industry.

The iterative calculations to determine the pack capacity and the electrode efficiency have been refined to arrive at the answer in fewer iterations; the standard 100 iterations provided by the Excel program is adequate and does not need to be extended to 1000 as was necessary for BatPaC 2.0.

EV Charging

In recognition of the need for rapid charging of all-electric vehicles a new worksheet has been added to BatPaC to address this requirement. A new chapter will be added to the BatPaC manual to discuss this worksheet and a draft of that chapter highlighted is included below:

5. High-Rate Charging of Electric Vehicle Batteries

Many new electric vehicles are being equipped for receiving high-rate charging. It has become standard even on the lowest priced Tesla S sedan, which now has a 70-kWh battery. Until recently, it was standard only on the more expensive 85-kWh model. Tesla and others are building charging stations throughout America and Europe that are capable of charging the battery at up to 135 kW of continuous power. Sufficient energy can be added to the Tesla Model S in 30 minutes for 180 miles of travel, about 68% of the range of the 85-kWh model. The USABC has shown interest in fast charging by tentatively listing a goal of charging 80% ΔSOC in 15 minutes for EV batteries with 45 kWh energy (EOL, ~53 kWh BOL).

To determine the maximum charging rate for a specific battery to be manufactured, extensive testing must be done. The calculations done in BatPaC approximately indicate the problems to be addressed in high-rate charging and estimate the costs of improving charging rate by reducing the electrode thickness and increasing the cell area.

5.1 Restrictions on the Charging Rate

The main restrictions on the charging rate are the following:

- The overpotential throughout charging must be safely below that at which lithium deposition would occur.
- The maximum power of the charging unit may further limit the charging rate.
- The battery temperature must not exceed 40°C.

Of these, the cell overpotential limit to avoid lithium deposition is the most restrictive for typical cell chemistries and EV battery designs. The charging rate may be improved while meeting the above restrictions by battery redesign to provide more cell area or by providing a more powerful charger, but often at higher cost.

5.1.1 Overpotential Limits

The area-specific impedance (ASI) of the battery cells is typically two to three times higher during continuous charging than on acceleration or regenerative braking. The overpotential needed for continuous charging is the sum of the overpotentials for (1) cell ohmic resistance in the electrolyte, (2) electrolyte salt concentrations, (3) positive electrode charge transfer and (4) negative electrode charge transfer. Of these, modeling has shown that the overpotentials for the electrode charge transfers, especially that for the negative electrode are the major contributors to the total [a].

Modeling studies at Ford Motor Company [a] of high-rate charging have shown that for 59.1-µm graphite negative electrodes and $Li(NiCoMn)O_2$ positive electrodes and for the configurations that are also typical of the default values in BatPaC, the avoidance of excessive overpotentials requires restricting the current density to about 4.2 mAh/cm^2 for charging to 67% of full capacity. This limitation on current density would apply for other positive electrodes and other electrode thicknesses. Additional charging could be done at reduced current densities such as imposed by constant voltage.

The maximum power of the charger may limit the charging voltage to a lower level than the limiting current density. Also, for some batteries it is advantageous to restrict the power at the charger to avoid excessive battery heating.

5.1.2 Battery Heating Limits

The high cell ASI values that result in high charging voltages also cause high rates of heating. This heating may be accommodated by efficient cooling and accordingly, BatPaC has been changed to call for cooling of 6 kW to be available for all EV batteries. Another way to accommodate the heat generation is to allow the battery temperature to rise to 40°C before restricting the charging rate. This approach can be enhanced by precooling the battery to 15°C. BatPaC has always assumed that the normal battery operating temperature is 15°C rather than a higher temperature to achieve the maximum service life of the battery and to accommodate long parking periods during summer without need for cooling. Typically, the use of the battery heat capacity accommodates an additional 15 to 60% as much heat as 6-kW cooling.

5.1.3 BatPaC Calculations for High-Rate Charging

To illustrate the characteristics of electric vehicle batteries during high-rate charging, four NMC-441 batteries were designed for different types of EVs (Table 5.1). The energy requirements, power and costs of these batteries differ considerably.

Table 5.1 Electric vehicle battery packs with NMC-441-graphite cell chemistry to illustrate high-rate charging characteristics

Battery Pack	**1**	**2**	**3**	**4**
EV Vehicle Type	Compact	Sedan	Sport Sedan	SUV
Range, miles	100	180	270	300
Energy usage, Wh/mile	200	250	250	350
Battery energy, kWh				
Total	23.5	52.9	79.4	123.5
Available	20.0	45.0	67.5	105
Battery pack power, kW				
10-s pulse	120	120	300	360
30-s pulse	93	93	231	278
Ratio V/U at full power, %	84.1	91.6	86.2	85.3
Electrode thickness, microns				
Positive	58	78	70	101
Negative	69	93	83	120
Price to OEM at 100 k/year, $	5,655	9,028	12,898	17,841

To calculate the capability of the lithium-ion EV batteries for receiving high-rate charging, a new worksheet, EV Charging, has been added to BatPaC and the results for the battery packs of Table 5.1 are illustrated in Figure 5.1. At the top of the worksheet, parameters relevant to charging are copied from the Battery Design worksheet. The maximum power of the charger is then added as new input. Also, a value for the maximum current density on charging of 4.0 mA/cm^2 is provided as a result of the modeling studies discussed above. Three cell ΔV values are then calculated based on (1) the maximum power of the charger, (2) the maximum current density limit to avoid lithium deposition, and (3) the maximum ΔV that avoids exceeding the temperature limit for the pack. The latter ΔV limit is calculated from the list of parameters directly below that limit. The C-rate for charging the first 60% SOC (from 15% to75% SOC) is next listed and it varies from 0.94 to 1.64, depending on the area and thickness of the electrode.

Rapid Charging of Electric Vehicles (EVs)				
Time for Charging	**Battery 1**	**Battery 2**	**Battery 3**	**Battery 4**
Battery capacity at C/3, Ah	75.7	171.3	299.2	351.5
Battery energy storage, Wh	23,529	52,941	79,412	123,529
Equivalent number of cells in series	84	84	72	96
Battery open-circuit voltage at 50% SOC, V	315.0	315.0	270.0	360.0
Battery open-circuit voltage at 20% SOC, V	299.5	299.5	256.7	342.2
Average battery Impedance during full discharge or charge, ohms	0.1734	0.1034	0.0460	0.0734
Charger power, kW	135	135	135	135
Maximum current density to avoid lithium deposition (<75% SOC), mA/cm2	4.0	4.0	4.0	4.0
Maximum cell ΔV at 20% SOC for full charger power, V	0.766	0.488	0.309	0.280
Maximum cell ΔV to avoid lithium deposition, V	0.256	0.257	0.260	0.254
Cell ΔV at which temperature exceeds maximum allowed, V	0.412	0.336	0.276	0.279
Initial battery temperature, oC	15	15	15	15
Maximum allowed battery temperature, oC	40	40	40	40
Maximum cooling rate, kW	6.0	6.0	6.0	6.0
Estimated heat capacity of battery, J/g-oC	0.85	0.85	0.85	0.85
Mass of battery pack less 50% of jacket mass, kg	155.0	291.9	432.9	642.5
Initial C-rate on charging, A/Ah	1.64	1.22	1.36	0.94
Limiting charging restriction (Charger, Li deposition, Temperature)	**Li deposition**	**Li deposition**	**Li deposition**	**Li deposition**
Total time charging 60% SOC (15 to 75% SOC), min	**22.0**	**29.5**	**26.4**	**38.1**
Total time charging 70% SOC (15 to 85% SOC, 82% useable), min	**26.9**	**36.1**	**32.3**	**46.6**
Total time charging 80% SOC (from 15 to 95% SOC), min	**34.2**	**45.9**	**41.1**	**59.3**
Total battery cost to OEM, $	**5,655**	**9,028**	**12,898**	**17,841**

Figure 5.1 Charging conditions for battery packs described in Table 5.1.

The limiting restriction on charging is shown on the next line in red (determined by the most restrictive overpotential calculated above) whether (1) the maximum power available from the battery charger, (2) the limiting current density to avoid lithium deposition, or (3) the temperature limit for the pack. For the battery packs and conditions demonstrated in Figure 5.1, avoiding lithium deposition is the most limiting constraint.

The time required to add 60% to the SOC varies from 22.0 to 38.1 minutes. To add an additional 10% SOC, the charging rate for that increment is reduced from the initial 4.0 A/cm^2 to 3.0 A/cm^2 and for a final 10% SOC (to a total of 95% SOC) the rate is further reduced to 2.0 A/cm^2.

The results of the high-rate charging are automatically transferred to the "USABC" worksheet, if the batteries are designated to be "EV" on the "Battery Design" worksheet. For other types of batteries, the times required for high-rate charging are left blank on the "USABC" worksheet.

[a] C. Chandrasekaran, "Quantification of Bottlenecks to Fast Charging of Lithium-Ion-Insertion Cells for Electric Vehicles", *Journal of Power Sources"*, 271 (2014) 622-632.

Summary of Results

It is believed that the improvements made in restricting the thickness of the electrode coatings have reduced the size of errors in estimating the cost and in the complexity of estimating the errors. As a result, the entire worksheet, Error Bar, has been eliminated and replaced by a simpler calculation at the bottom of the Summary of Results worksheet.

USABC Data

The United States Battery Consortium (USABC) is especially interested in key battery performance parameters, and these are summarized on this new worksheet for the seven batteries designed on a standard BatPaC spreadsheet.

Thermal Modeling

Adjustments were made to the calculation of the heat generated in the battery to better account for the differences in the vehicle weight and expected driving cycles as reflected in the energy requirement for the vehicle (Wh/mile), an input parameter for the Battery design worksheet.

Cost Input

In providing cost inputs for the section "Battery Assembly Costs" the following two changes were made:

NMP Solvent Recovery

A process model was used to estimate the cost of NMP recovery. The capital cost for the NMP recovery process has been revised to $5M (previously $3M). This capital cost does not include the cost of the dryer since it is already included in the cost of the coater-dryer. The labor required for the NMP recovery process has been revised to 10,800 hours per year (previously 14,400), which consists of 1 engineer working 8 hours per day, and a semi-skilled worker on duty 24 hours per day.

Dry Room Management

The capital cost for the dry room management includes the cost of the enclosure, floors and ceiling, and the equipment needed to provide and condition the air flow to and from the dry room. A dedicated model was set up to study the energy consumed and cost of operating the dry room. This model was used to estimate the capital cost of the dry room in the baseline plant. It has been revised to $6M (previously $20M). The labor requirement for operating the dry room was revised to 7,200 manhours per year (previously 14,400), which consists of 1 engineer working 2 hours per day, and a semi-skilled worker on duty 12 hours per day.

Manufacturing Cost Calculations

Corrections were made in calculating the costs of thermal control devices to the battery, which adds slightly to the cost.

Price of Cells and Modules

In addition to estimating the prices of entire battery packs, BatPaC 2.0 estimated the price of providing only modules of cells not including the battery enclosure. BatPaC 3.0 goes one step further and also calculates the price for providing only the cells without the module and pack hardware. The resulting values are added to the Summary of Results and a breakdown of these costs is provided in the USABC Data.

Worksheets Module and Batteries

These worksheets provide schematic designs to assist in assigning costs to the various design requirements, and are not intended to provide tested design features. A battery design feature added in the new version of BatPaC and illustrated in these worksheets is the provision for venting gas buildup, for which a section will be added to the Manual as shown in draft form below:

2.3.3. Venting Gas Buildup

Progress is being made in developing lithium-ion cell chemistries that reduce the likelihood of high temperature excursions caused by runaway reactions resulting in rapid gas build-up. At the present time, lithium-ion batteries are being designed to minimize the injury to vehicle passengers and the damage to the vehicle in the event of rapid release of gases.

The BatPaC model estimates the cost of lithium batteries that will be the most successful in meeting battery cost targets that are compatible with electric-drive vehicles capturing a large fraction (>30%) of the vehicle market. Thus, it is assumed that the release of gases from rapid oxidation reactions within the batteries will be rare events and that provision for such occurrences will be inexpensive. We do not attempt to design batteries that will certainly solve the problem of pressure build-up, but we merely suggest design strategies that show promise of meeting this challenge at low cost and assume that battery manufacturers will achieve this goal at about the same cost.

In the event of excessive pressure, gas will be released from the BatPaC cells by the unsealing of the cell pouch at the terminal seal at the back end of the module (Fig. 2.5). A gas passage is provided beyond the end of the cell terminals. This passage permits gas to be released through pressure relief disks on the module wall and the thermally insulated pack housing (Fig. 2.5 and 2.7). The gas is released to a channel that is less than 30 mm from the escape point at the cell, and which directs the blast down to the street directly beneath the battery, which is presumed to be located on the floor of the vehicle such as under the rear seat.

This method of providing for gas release adds very little to the volume of the battery, only the space that is occupied by the gas passage between the cell terminals and the back of the module (approximately 6 mm). However, a flow passage of 20-to 30-mm width must be provided outside of the battery pack next to the back of the modules and on both sides of the module for larger batteries with two rows of modules. The cost of providing for the sudden release of gas is expected to be small if the proposed mechanism or a similar simple approach is shown to be satisfactory.

In the latest version of BatPaC, provision has been made for the additional volume of the battery and $3.00 per module is added to the cost of the pack for this provision.

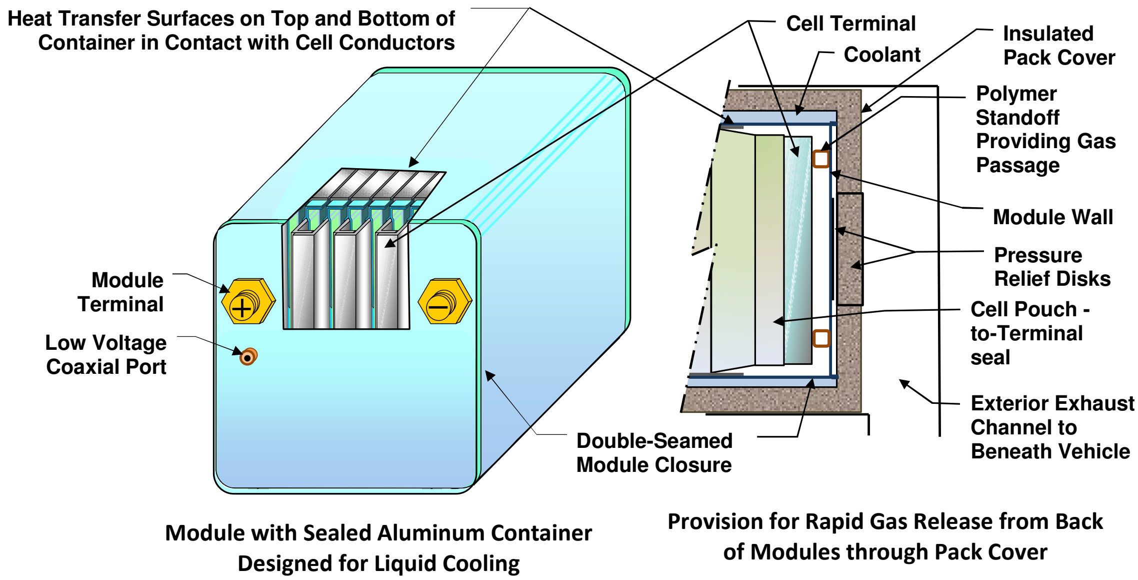

Figure 2.5. Module with hermetically sealed aluminum container for batteries utilizing a liquid thermal management system showing gas-release system